The Nucleus ***52****, No. 4 (2015) 146-150*

www.thenucleuspak.org.pk

The Nucleus

ISSN 0029-5698 (Print)
ISSN 2306-6539 (Online)

Evaluation of Optimal Top Coat Thickness in Composite LTA/YSZ Thermal Barrier Coating by Comparative Stress Distribution using Finite Element Method

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ARTICLE INFO

Article history :
Received : 12 October, 2015
Revised : 27 October, 2015
Accepted : 27 October, 2015

Keywords :
TBC
FEA
LTA/YSZ
Ceramic coating
Stress distribution

ABSTRACT

Demand of high operating temperature in gas turbines for better efficiencies has forced researchers to explore novel materials with improved thermal properties. In this regard, $LaTi_2Al_9O_{19}$ (LTA) is recently declared as a brilliant candidate for thermal barrier coatings (TBCs). Owing to potential advantages like high temperature stability & low thermal conductivity, researchers are striving to use it for modern gas turbines. An innovative concept of composite ceramic coating (LTA+YSZ) has been introduced to achieve improved set of thermal & mechanical properties. In this paper, a finite element analysis (FEA) has been employed to observe stress scattering with relatively varying thicknesses of compositional ceramic coats using commercially available software ANSYS. Optimum set of variables has been proposed based on the associative stress state data calculated from FEA results. Radial & axial stresses (σ_{xx}, σ_{yy}) are ascertained for composite system and ultimate values of stress are offered for comparison on quantitative grounds. Elastic strain energy stored in TGO is determined based on FE results to estimate the structural reliability of TBC. Conclusively, trend reveals that both radial & axial stresses are respectively proportional to increasing & decreasing thickness of YSZ. Comparing elastic strain energies, maximum life is evaluated in 1:4 for YSZ: LTA which shows that composite layer TBC system have improved stability than single layer system as reported in literature.

1. Introduction

Thermal barrier coatings (TBCs) are frequently applied as shielding coatings for modern power engineering systems to enhance thermal efficiency and performance [1-5]. Ever increasing demand to enhance the efficiencies of gas turbines have proved to be a major motivational element to boost the technology of ceramic coatings by innovative configurations and manufacturing methodologies for subsequent microstructure's improvement for better performance. Presently, zirconia stabilized by yittria (YSZ) is the state of the art industrial grade top coat material for TBC systems, that sustains at temperatures below 1200 °C [2,5,6].

In general, ideal TBCs must have capability of phase stability between operating temperature & room temperature, good sintering resistance at elevated temperature, low thermal conductivity, high fracture toughness and most important to have an ability of coating formation with stochiometric, consistent and well controlled structure [7-9]. No single material is declared that qualifies all parameters commercially.

Due to operating temperature limitation T<1200 °C of YSZ, substitute materials for top coat were worked out for modern application such as in gas turbines. The aim behind such substitution is achieving higher efficiencies. During the last few years, variety of ceramic coatings has been suggested as alternatives. These novel compositions comprises of oxides, doped zirconia [10-11], pyrochlores [12-14], aluminates [15-17] and perovskites [18, 19].

In recent past, lanthanum-titanium-aluminum oxide [$LaTi_2Al_9O_{19}$] (LTA) has been proposed as top coat material due to its improved thermal properties at higher temperature up to 1500°C [20-23]. Achievement of Lower thermal conductivity in LTA is made by its crystallographic sites [22].

Researchers, over the period of time evaluated LTA from different aspects including thermal & mechanical properties and its stability at elevated temperature [20-23]. A finite element (FE) based study has been performed for composite YSZ/LTA TBC systems with variable thicknesses of top coats. For structural reliability estimation, elastic strain energy in each case is calculated to evaluate stress states in thermally grown oxide (TGO) for all cases. Findings are analyzed with earlier investigations on failure of TBCs driven by thermal expansion mismatch.

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In this work, composite ceramic coating (LTA+YSZ) has been introduced to get good combination of thermal & mechanical properties. Stress scattering with relatively varying thicknesses of compositional ceramic coats was observed through Finite element analysis (FEA) using commercially available software ANSYS.

2. Finite Element Analysis

In finite element (FE) model, round disc sample is take in to account hat permits the problem to be shaped into a 2-D axi-symmetric case in axial & radial directions as depicted in Fig. 1. There are five layers in composite ceramic TBC system. An extra layer is deposited at the top of YSZ. Thicknesses of substrate, bondcoat and TGO are 2mm, 120µm and 7µm respectively. Thickness of top coat (varying parameter) in double-ceramic-layer coating is categorized as shown in Table 1. Two-dimensional element PLANE223 (coupled field) has been used for a coupled thermo-mechanical FE analysis. Element PLANE223 has versatility in respect of four degrees of freedom associated with each node. It has total eight nodes so its behavior in respect of computation is well engineered. Mapped grid has been selected for easy computation.

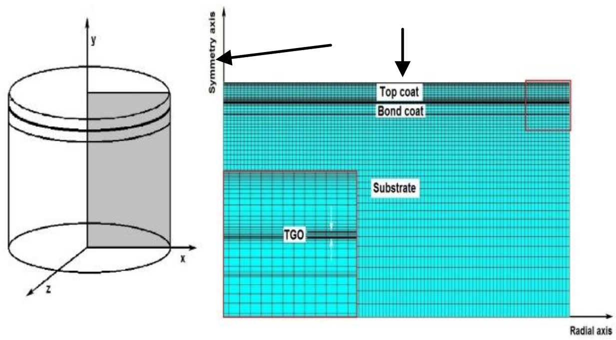


Fig. 1: Geometric model and FE mesh

There are approximately ~30000 elements that depend on thickness of composite ceramic coats. TGO is finely meshed due to its little thickness. Similarly, surrounding regions around TGO are finely meshed to improve their response (stress distribution) against loading scenario.

There are five materials in the model: Ni-based super alloy substrate, NiCrAlY bond-coat, Al_2O_3 i.e. TGO, Yittria stabilized zarconia and Lanthanum-titanium-aluminum oxide as ceramic topcoats. Different temperature dependent mechanical and thermal properties of these materials used in FEA acquired from published data [22, 24].

Symmetric boundary conditions are used due to axisymmetric arrangement of the model. Boundary conditions or constraints have major role in simulation because the most stresses are caused by settlement of constraints and thermal effects (arising from temperature differences). A uniform thermal gradient is applied through cooling from 1050°C to room temperature. It has been assumed that there are no stresses at 1050 °C.

Table 1: Classification of cases as a function ofTop coat thickness in double-ceramic layer TBC system

Case No	YSZ (µm)	LTA (µm)
1	40	360
2	80	320
3	120	280
4	160	240
5	200	200
6	240	160
7	280	120
8	320	80
9	360	40

It was assumed that layers of TBC are homogeneous and isotropic [25]. The upper most surface of TBC is exposed to hot gases and it has been assumed that this surface is free of any mechanical constraint. Convection is applied on the top surface of the model while thermal insulation is considered at the base of the sample. Creep and phase transformation which can cause thermal stress changes are expected to be dormant during the analysis [24]. After applying above mentioned boundary conditions, analysis was conducted to assess the stress distribution in the considered TBC system. Maximum radial & axial stresses for all considered cases are ascertained and presented in subsequent sections.

3. Findings and Discussions

3.1 In-plane Stresses

For composite coating systems, variation in maximum tensile radial stress as a function of top coat thickness is depicted in Fig. 2a.

These radial stresses are mostly found at the union coat/TGO border close to edge of the sample in all considered cases. It is clear from the fig that maximum tensile in-plane stress increases by subsequent increase in YSZ with relative decrease in LTA thickness. A sudden drop in stress value is observed in case-2 (YSZ=80µm) and after that linear increase is perceived observed for onward simulations.

Fig. 2b shows residual compression stresses in duplex top coat TBC system with considered TGO thickness. Cooling stresses are produced due to mismatch in the thermal expansion coefficients between oxide layer & bond coat when a stress free-state is assumed at the higher temperature side. Fig. shows that compressive stresses for TBC increase uniformly with the increase & decrease in YSZ& LTA thicknesses respectively. A difference of 150 MPa exists between Case-1 and Case-9.

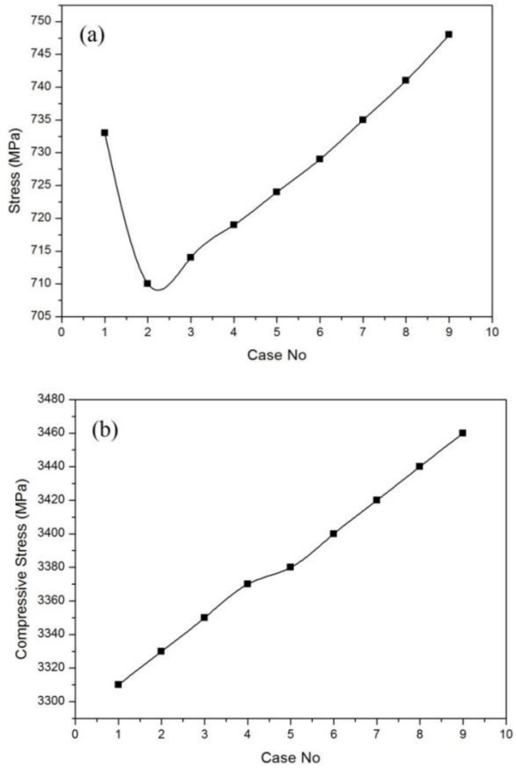


Fig. 2: In plane tensile (a) & compressive (b) stress in YSZ+LTA coating systems as a function of top coat thickness

3.2 *Out of Plane Stresses*

For composite coating systems, variation in maximum out of plane tensile stress with varying thickness is depicted in Fig. 3a. Figure states that normal tensile stress drops with the increasing thickness of YSZ. These maximum stresses are less harmful to critical interface as compared to in-plane stresses prevailing in important areas within TGO and at interface areas. However, tensile stresses in TBC normal to the interface are detrimental in crack initiation and subsequently its dissemination during tenure of thermal contact. Eventually it can lead to instability of TBC system. Likewise reservations comprised in literature that crack developed in LTA layer causing chipping spoliation of the whole TBC (YSZ+LTA) [26].

Variation in axial compressive stresses in composite coatings as depicted in Fig. 3b illustrates that compressive stresses (axial) is in decreasing order with increasing thickness of YSZ considered in this study. Normal compressive stresses found in substrate at the outside edge of the sample close to edge of substrate/bondcoat in all considered cases.

Literature reveals that oxides at substrate/bond coat edge are of usually non-alumina form [27, 28]. This will results in poor interface properties and thus any stress profile in this locality will also be of vital importance.

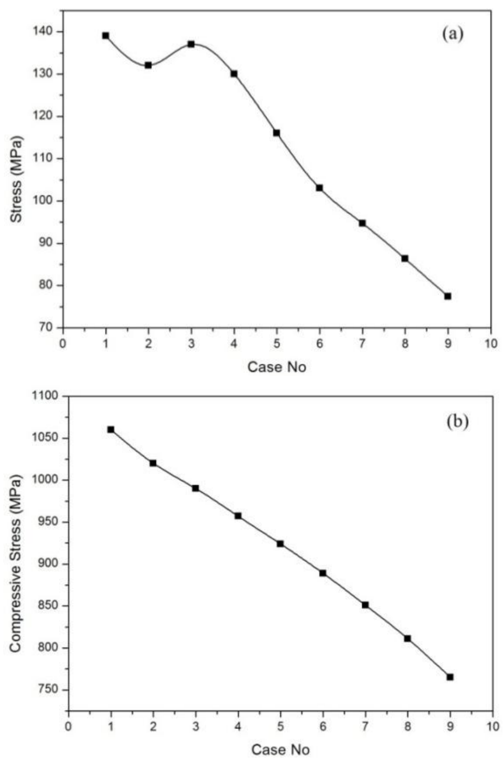


Fig. 3: In axial tensile (a) & compressive (b) stress in YSZ+LTA coating systems as a function of top coat thickness

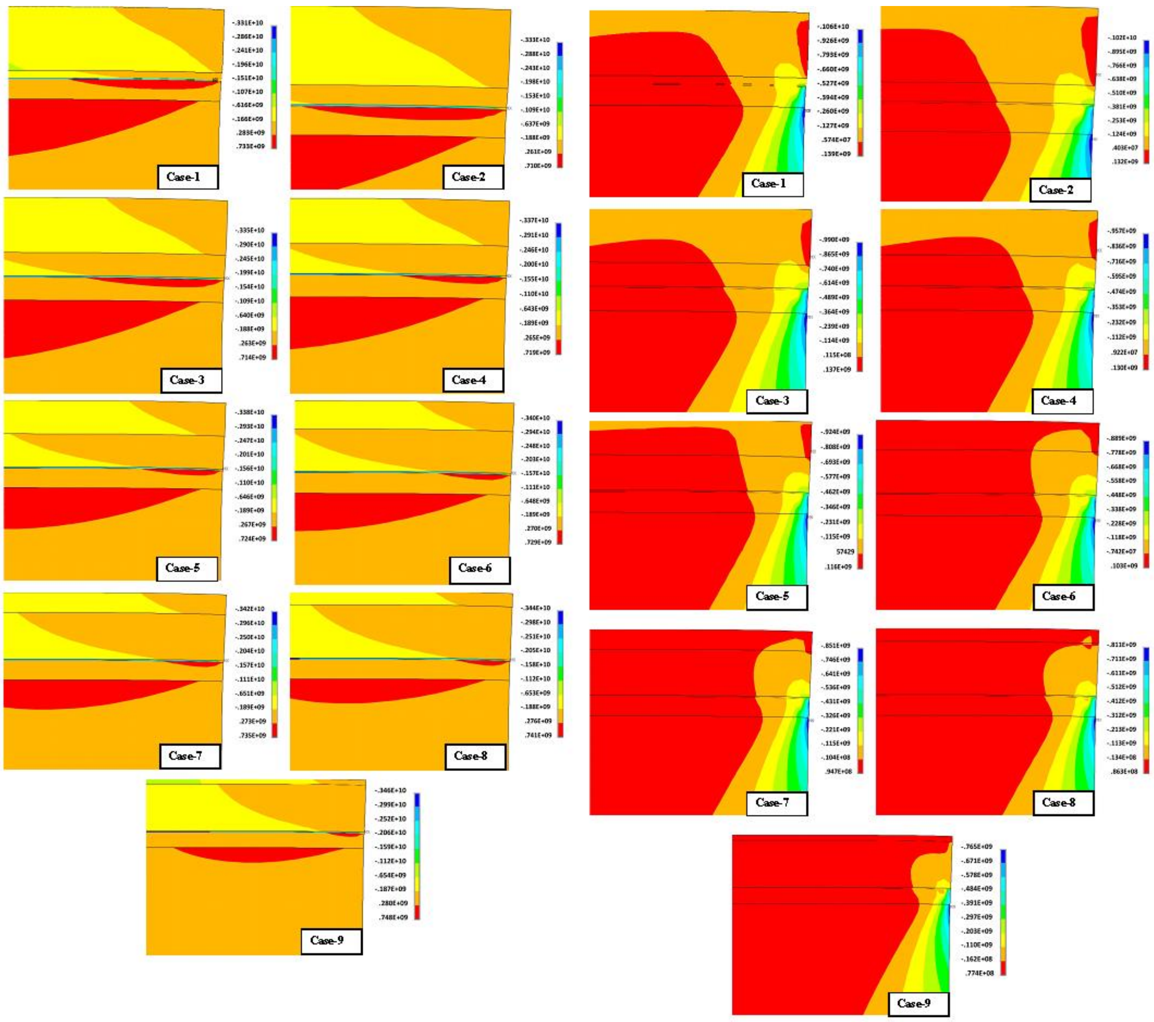
Radial & Axial Stress status is further explained with the help of contour plots of radial & normal stress for variable top coat thickness cases presented in Fig. 4. As shown in Fig. 4, peak normal axial tensile stress in the composite coatings system lies close to periphery of the specimen adjacent to the boundary.

3.3 *Elastic Strain Energy Stored*

The stability of the Thermal Barrier Coatings is managed by the TGO`s energy density and analyzed by manipulating overall elastic store energy per unit area [29]. Elastic energy per unit area stored in unbuckled film (G_o) has proportional relationship with oxide thickness h_{ox} and radial compressive stress and is stated in this fashion [30].

$$G_o = \frac{(1-v_{ox})}{E_{ox}} h_{ox} \sigma_{ox}^2$$

Where V_{ox} & E_{ox} are corresponding poisson’s ratio & young modulus of alumina oxide (TGO). Usually for Al_2O_3 oxide film, G_o $\approx 1.925\times10^{-12}$.TGO failure is possible if G_o exceeds Γ_o, where $\Gamma_o$is the fracture toughness of the YSZ/TGO edge [31]. For the assessment of TBC’s structural integrity, elastic store energy G_o is determined from FE results calculated for TGO with different set of composite layer thicknesses. Stress profile and low elastic stored energy in composite coating system complies with the previous findings [22].



(a) (b)

Fig. 4: Contour plots of (a) radial stress (σ_{xx}) & (b) normal stress (σ_{yy}) distribution in YSZ + LTA coating as a function of top coat thickness

The outcomes for elastic store energy G_o are shown in Fig. 5. It shows that store energy value is increasing with the increase of YSZ with respect to LTA in composite top coat. Study suggests optimizing the YSZ/LTA thicknesses to achieve the optimum performance with respect to high temperature, stability and thermo-mechanical behaviour of the TBC.

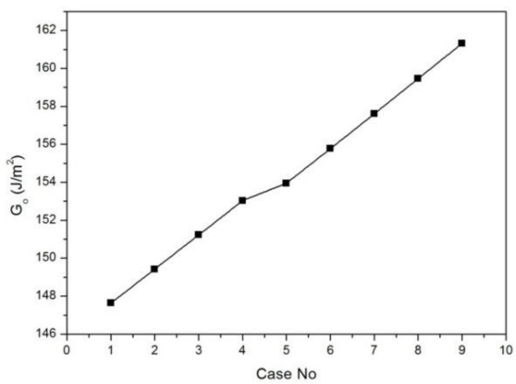


Fig. 5: G_0 within TGO for double layer coating (YSZ+LTA) systems

4. Conclusion

Concisely, the current work analyzes the stress response of double layer TBC system under thermal loading scenario. Comparative analysis of the stress distributions based on numerical study has been carried out for YSZ+LTA TBC system for different top coat thickness (40~360μm). It has been observed that radial stresses increase with the increase of YSZ thickness in composite layer. However, a drop in axial stresses has been observed conversely. Keeping in view the stress state and potential advantage of using composite top coat with dual benefits of high temperature stability from LTA and thermal expansion properties from YSZ, study propose the use of composite YSZ+ LTA coating with 1:4 ratio of YSZ: LTA.

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